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# NUMERICAL MODELING OF TWINNING IN GaAs CRYSTALS DURING SPACE GROWTH PROCESS

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## ABSTRACT

A quantitative model for prediction of twin formation during the space Gallium Arsenide (GaAs) crystal growth has developed. Twinning is an important defect in advanced semiconductor crystals such as GaAs and InP. The deformation twins are formed in the GaAs crystal during its growth processes from the melt in the space. The thermal stresses during the crystal growth are the primary cause of deformation twinning formation. The thermoelastic stresses generated in the grown crystals are calculated from two-dimensional finite element analysis. In the present study, a new computer simulation model is developed for calculating the stress distributions of each twin systems in the GaAs crystals grown at different growth orientations from the melt. This investigation is expected to further the understanding of twinning formation and provide valuable information about the growth parameters' effects on twinning formation in crystals for growing low defect GaAs crystals.


## 1. INTRODUCTION

GaAs single crystals are becoming an important material in semiconductor device technology. Due to its high mobility, saturated drift velocity and the ability to produce semi-insulating substrates, GaAs semiconductor devices become more important as compared to silicon. However, the presence of defects (twins and dislocations) in GaAs crystals are much more than that in Silicon crystals. It is well known that the crystal defects in these materials adversely affect the life time and performance of these devices [1]. For example, Brantley and Harrison [2] have observed that the degradation rate in diffused electroluminescent diodes increased by an order of magnitude. These persuasive results suggest that commercial viability of high-speed electronic and photonic devices and circuits are strongly dependent on the availability of low defect GaAs and InP crystals. By and large, wafer size and electrical property requirements can be met by the present manufacturing state of the art. However, cost effective high volume production of low defect density crystals still remain a key problem for semiconductor community.

Bulk growth of electronic and photonic crystals is entering a new era of increased emphasis on intelligent processing. Combination of process model with advanced sensors and controls, future equipment such as the Programmable Multi-Zone Furnace may dramatically improve the resulting crystal quality. The virtual elimination of convection in the melt during processing yields only diffusion-controlled axial segregation. Even though much attention has gone into the thermal-fluid modeling of solidification to understand the complex physical and chemical transport phenomena that prevail during the processing of materials, modeling of crystal defect generation is sparse during crystal growth for understanding the relationship between the generation, motion and multiplication of dislocations and twins in the crystal and processing conditions.

Presently no satisfactory general understanding exists which allows the bulk growth of crystal having low crystal defect density with quality desired for future applications in the field of microelectronics and optoelectronics. Formation of deformation twins depend strongly on the temperature gradient present during crystal growth, non-skoichiometry of the melt, and facet growth. An improved understanding of the twin formation in GaAs crystals can be accomplished through a good quantitative modeling of shear stresses in the twinning systems for different growth orientations from the melt. Furthermore, this model can be employed for optimizing the growth configurations and parameters with respect to twin formation in GaAs crystals. In the following section, the basic simulation procedure for studying the twin growth is summarized. Results of numerical simulations are presented and analyzed in Section 3. Finally, the last section presents a discussion of the simulation results.

## 2. SIMULATION MODEL OF TWINNING FORMATION

In the crystal growth processing which is shown in Fig. 1, a cylindrical ingot with typical curved interface is solidified from the melt. Modeling of solidification during crystal growth is rather complex. Several time and length scales spanning many orders of magnitude are simultaneously responsible for setting the flow, thermal and solutal fields. Other complicating effects are time dependency, multi-dimensionality, flow transition, and the presence of unknown solidification fronts. A detailed modeling of such complex phenomena is not the objective of this study. However, the temperature fields which are used to model the residual stress state and twin formation in the crystals are obtained from a less complex heat transport model.

The temperature gradient fields in the crystal during growth processes is obtained from a general purpose finite element code FIDAP [3], enhanced specifically for simulating crystal growth processing [4]. The temperature gradients induces a thermal stress field in the growing crystal as a result of spatially inhomogeneous thermal contraction. Temperature distribution are used for calculating the stress components in the crystal. In the model, the growing crystal ingot is assumed to be an axisymmetrical solid (Fig. 1). If u and w are displacement components in the r and z directions, respectively, then the strain components in the cylindrical coordinates are

$$\epsilon_{rr} = \frac{\partial u}{\partial r},\ \epsilon_{\theta\theta} = \frac{u}{r},\ \epsilon_{zz} = \frac{\partial w}{\partial z},\ \epsilon_{rz} = \frac{1}{2}\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial r}\right). \tag{1}$$

By assuming GaAs crystal as an elastically isotropic material, the stress-strain relations are:

$$
\begin{Bmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \\ \sigma_{zz} \\ \sigma_{rz} \end{Bmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & \nu & 0 \\ \nu & -\nu & \nu & 0 \\ \nu & \nu & 1-\nu & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{\nu} \end{bmatrix} \begin{Bmatrix} \epsilon_{rr} & -\alpha\Delta T & -\epsilon^{pl}_{rr} \\ \epsilon_{\theta\theta} & -\alpha\Delta T & -\epsilon^{pl}_{\theta\theta} \\ \epsilon_{zz} & -\alpha\Delta T & -\epsilon^{pl}_{zz} \\ \epsilon_{rz} & -\epsilon^{pl}_{rz} & \end{Bmatrix} \tag{2}
$$

where subscripts rr, $\theta\theta$ and zz refer to the r, $\theta$ and z coordinate system of Fig. 1. Based on Eqs. (I-2) and the principle of virtual work, a nonlinear finite element equation for the thermal viscoplastic problem of quasi-steady-state crystal growth in terms of displacement fields is given as [5]

$$
[K_s(T)]\{U\} = \{F_p\} + \{F_T\} + \{F_\sigma\} + \{F_b\} = \{F\}, \tag{3}
$$

where $[K_s(T)]$ is the stiffness matrix, which is a function of temperature; U represents the nodal displacements u and w; and the terms on the right hand side are load vectors due to plastic strain ($F_p$), temperature gradients ($F_T$), surface traction ($F_\sigma$) and body forces ($F_b$), respectively.

The thermal stress calculation are performed in cylindrical coordinate system in which z axis is assigned to be a growth axis in this simulations, either [0 0 1] or [1 1 1] as shown in Fig. 1. In the simulations, x//[l 0 0], y//[0 I 0] and z//[0 0 1] are chosen in the case of crystal growth direction of [0 0 1], and if the growth direction is [1 1 1], x//[l -2 1], y//[I 0 -1] and z//[1 1 1] are selected. The cylindrical stress components $\sigma_{rr}, \sigma_{\theta\theta}, \sigma_{zz}$ **and** $\sigma_{rz}$ are transformed into Cartesian coordinate system by use of the stress transformation tensor, $\sigma_{i'j'} = \sigma_{kl}\, l_{i'k}\, l_{j'l}$ , where $l_{i'k}$ **and** $l_{j'l}$ are direction cosines, (i,j,k,l = 1,2,3), $i'j'$ and kl are stress tensor in Cartesian and cylindrical coordinate systems, respectively.

The major mechanism by means of twins is introduced during crystal growth caused by excessive thermal stresses. GaAs crystals have crystal structure of diamond. The twining plane in the diamond cubic case is {111} and twinning directions are <112>. There are a total of 12 twin systems that, can be considered in the present crystal system [6]. Those 12 permissible twin system are listed in Table 1. Formation of twins depends on the magnitude and directions of the stresses on twinning systems. Necessary condition for twinning is that the shear stress resolved on the twinning plane and in the twinning direction shall reach the critical resolved shear stress (CRSS) which is characteristic of the crystal. A local coordinate system (x', y', z') is defined for calculation of resolved shear stress (RSS) in each twinning system in which twining direction is along x', y' is normal to the twin plane, and z' is parallel to cross product of these vectors. The global stress tensor in Cartesian coordinate system at the position of the twin is transformed into the coordinate system of twin by use of the stress transformation tensor, where $\sigma_{i'j'}$ and $\sigma_{kl}$ are stress tensor in local and global coordinate systems, respectively. The RSS acting on the 12 twinning systems are then calculated using this model.

| Twinning System | Twinning Plane | Twinning Direction |
|---|---|---|
| 1 | 1 1 1 | -1 -1 2 |
| 2 | 1 1 1 | 1 -2 1 |
| 3 | 1 1 1 | 2 -1 1 |
| 4 | 1 -1 -1 | 2 1 1 |
| 5 | 1 -1 -1 | 1 2 -1 |
| 6 | 1 -1 -1 | -1 1 -2 |
| 7 | -1 1 -1 | 1 2 1 |
| 8 | -1 1 -1 | -1 1 2 |
| 9 | -1 1 -1 | -2 -1 1 |
| 10 | -1 -1 1 | 1 -2 -1 |
| 11 | -1 -1 1 | 2 -1 1 |
| 12 | -1 -1 1 | 1 1 2 |

Table 1. The 12 permissible twinning systems for GaAs.

## 3. RESULTS AND DISCUSSIONS

A GaAs ingot grown by a vertical Bridgman method is used as a numerical example for investigation of twin formation in the crystal using the crystallographic model. Details of GaAs crystal ingot is shown in Fig. 1. The temperature gradient fields and the solid-meld interface (melting point of GaAs, 1511 K) shape are shown in Fig. 2. The average temperature gradient is about 5 K/cm for the GTE experimental case [4]. The radius of the ingot is 1.27 cm, and the length is about 4 cm. The growth rate is 0.0005 cm/s.

Twin formation depends on the magnitude and direction of resolved shear stress on twin systems. Effect of crystal growth direction on defect concentration has been investigated for the [0 0 1] and [1 1 1] pulling orientations using the temperature distribution obtained from a finite element code FIDAP. The effect of temperature gradient along the growth orientation on twin formation in each twinning system has been studied, and resolved shear stresses on (1 -1 0) plane along the growth orientation of [0 0 1] near the center (r = 0.1 cm), the middle (r = 0.6 cm), and the edge (r = 1.2 cm), of the wafer for (-1 -1 1)[1 1 2], (-1 1 -1)[-1 1 2] and (-1 1 -1)[-2 -1 1] twin systems with larger RSS is shown in Figs. (3a-3c). Fig. 4 shows the resolved shear stresses on the plane between (1 0 -1) and (1 -2 1) (in Fig. 1b) along the [1 1 1] growth orientation near center, the middle, and the edge of the wafer for (a) (-1 -1 1)[1 1 2], (b) (-1 1 -1)[-1 1 2] and (c) (-1 1 -1)[-2 -1 1 ] twin systems which have larger RSS. It can be seen from Fig. 3 that resolved shear stresses near the center of the wafer are much greater than that near the midway and edge of the wafer along the growth orientation of [0 0 1]. On the other hand, Fig. 4 shows that resolved shear stresses near the edge of the wafer are much greater for the crystal growth orientation of [0 0 1].

Resolved shear stresses on planes along both the [0 0 1] and [1 1 1] pulling orientation (Figs. 3-4) for twelve twinning system show that the maximum shear stresses are always located near the top of the crystal. Therefore, distribution of resolved shear stresses on the (0 0 1) GaAs wafer near the top of the crystal are studied for each twinning system along the growth orientation of [0 0 1] and shown in Fig. 5 for twin systems (a) (-1 -1 1)[1 1 2], (b) (-1 1 -1)[-1 1 2] and (c) (-1 1 -1)[-2 -1 1]. Fig. 6 shows the stress contour lines of resolved shear stresses on (1 1 1) plane for (a) (-1 -1 1)[1 1 2], (b) (-1 1 -1)[-l 1 2] and (c) (-1 1 -1)[-2 -1 1] twin systems in the GaAs wafer for crystal grown along [1 1 1] pulling orientation. It is found that there are only two kinds of shear stress distribution patterns in the wafer for the 12 twinning systems. One is two-folds symmetric and the other is four-folds symmetric. For each twinning plane, there are always two twinning directions having two-folds symmetric stress distribution and one twinning direction having four-folds symmetric. For the crystal grown along the [0 0 1] pulling orientation, the largest shear stress of about $4x1O^5$ Pa, in twin systems is all located near the center of the wafer. The twinning systems having maximum value of stress are the twinning systems leaving four-folds symmetric stress distribution pattern.

Fig. 6 illustrates that largest resolved shear stresses in the (1 1 1) GaAs wafer grown along [1 1 1] orientation appears normal to the direction lying at 45° to the [1 0 -1] and [1 -2 1] directions on the wafer. Fig. 6 shows that the large portion of the largest resolved shear stresses ($2x1O^5$ Pa) in the wafer occur near the edges and the middle. If the CRSS for GaAs is less than calculated largest resolved stresses, no twinning will occur. Otherwise, twinning could occur in any twinning system as long as the RSS in this twinning system are greater than the CRSS. Since the CRSS for the GaAs is not available at present, we will present the contour plot of the CRSS which shows the distribution of possible formation of deformation twins in the crystal. Higher RSS indicates larger possibility of twinning.

## 4. CONCLUSION

A numerical model for calculating RSS in the twinning system of GaAs crystals has been developed for predicting the possible formation of deformation twinning during the growth of GaAs crystals. The calculated RSS in the grown crystal shows a strong dependence on the temperature profile and growth orientation. If the CRSS for GaAs is less than the RSS, no twinning will be generated. Otherwise, twinning could be generated in any twinning system.

Numerical models of RSS such as the one presented here, may provide valuable information for growing GaAs crystals with few deformation twins through the control of furnace temperature profile and pulling orientation during crystal growth in microgravity environment.

## 5. REFERENCES


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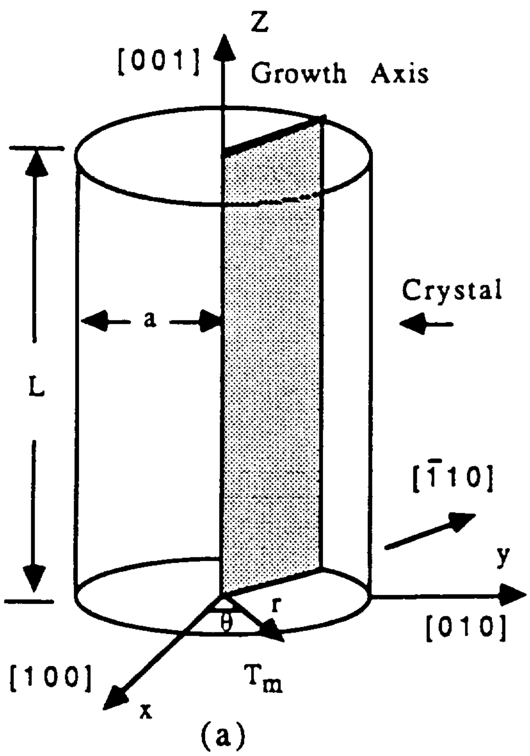


Fig. 1. Coordinate system of the crystal pulling along (a) the [0 0 1] and (b) the [ 1 1 1] orientation during crystal growth, where T is the melting point on the solid-melt interface of the crystal.

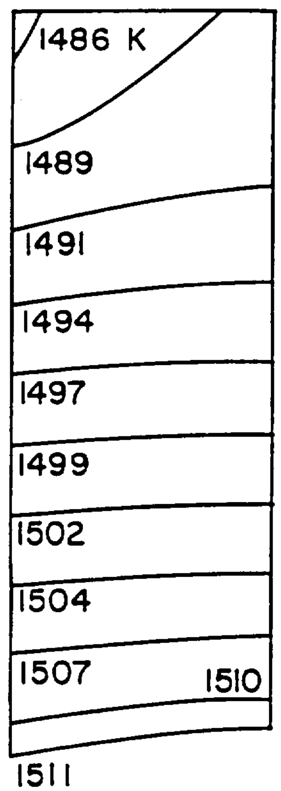


Fig.2. Temperature distribution in the crystal.

(a)

(b)

(c)

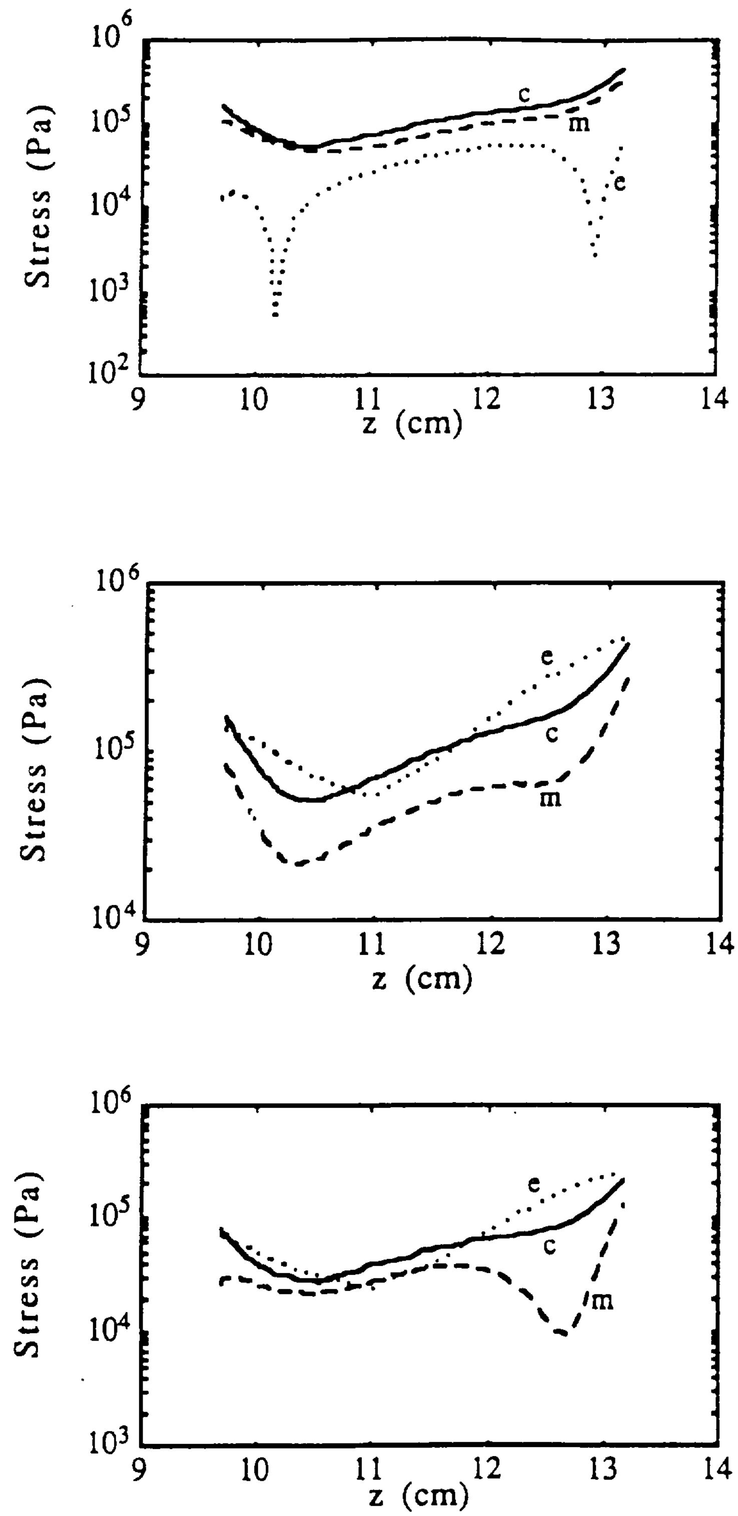


Fig. 3. Resolved shear stresses on 91 -1 0) plane along the growth orientation near the center, the middle, and the edge, of the wafer for (a) (-1 -1 1)[1 1 2], (b) (-1 1 -1)[-1 1 2], and (c) (-1 1 -1)[-2 -1 1] twin systems.

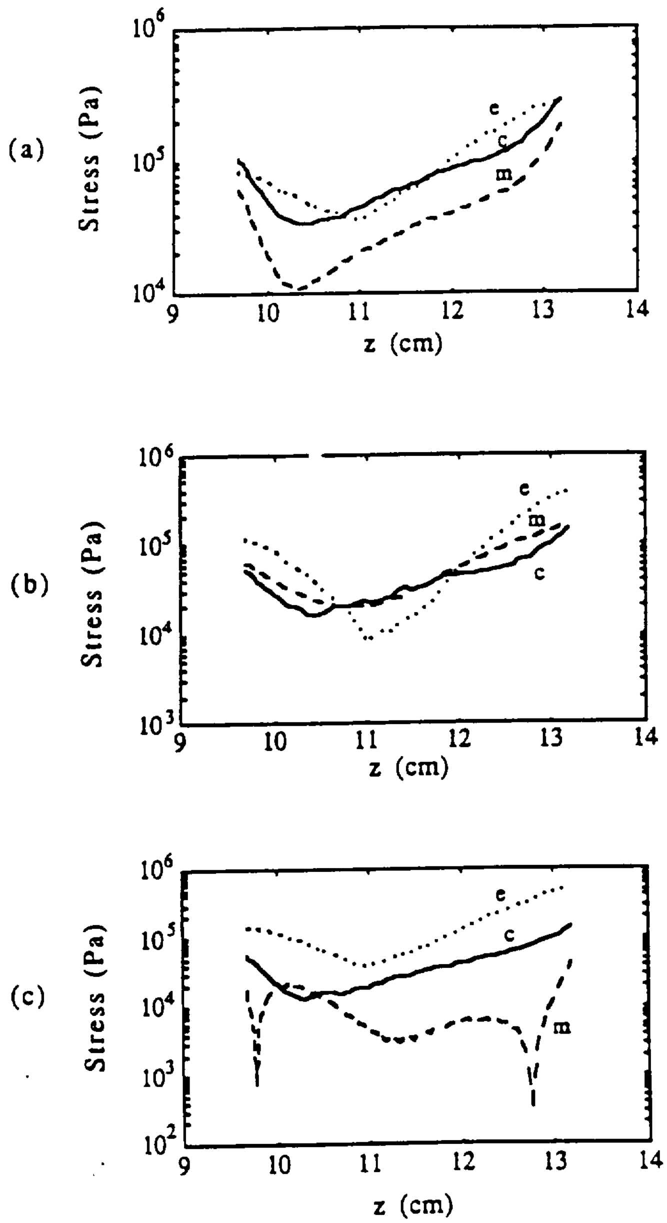


Fig. 4. Resolved shear stresses on the plane between (1 0 -1) and (1 -2 1) (as shown in Fog. 1b) along the [1 1 1] growth orientation near the center, the middle, and the edge of the wafer for (a) (-1 -1 1)[1 1 2], (b) (-1 1 -1)[-1 1 2], and (-1 1 -1)[-2 -1 1] twin systems.

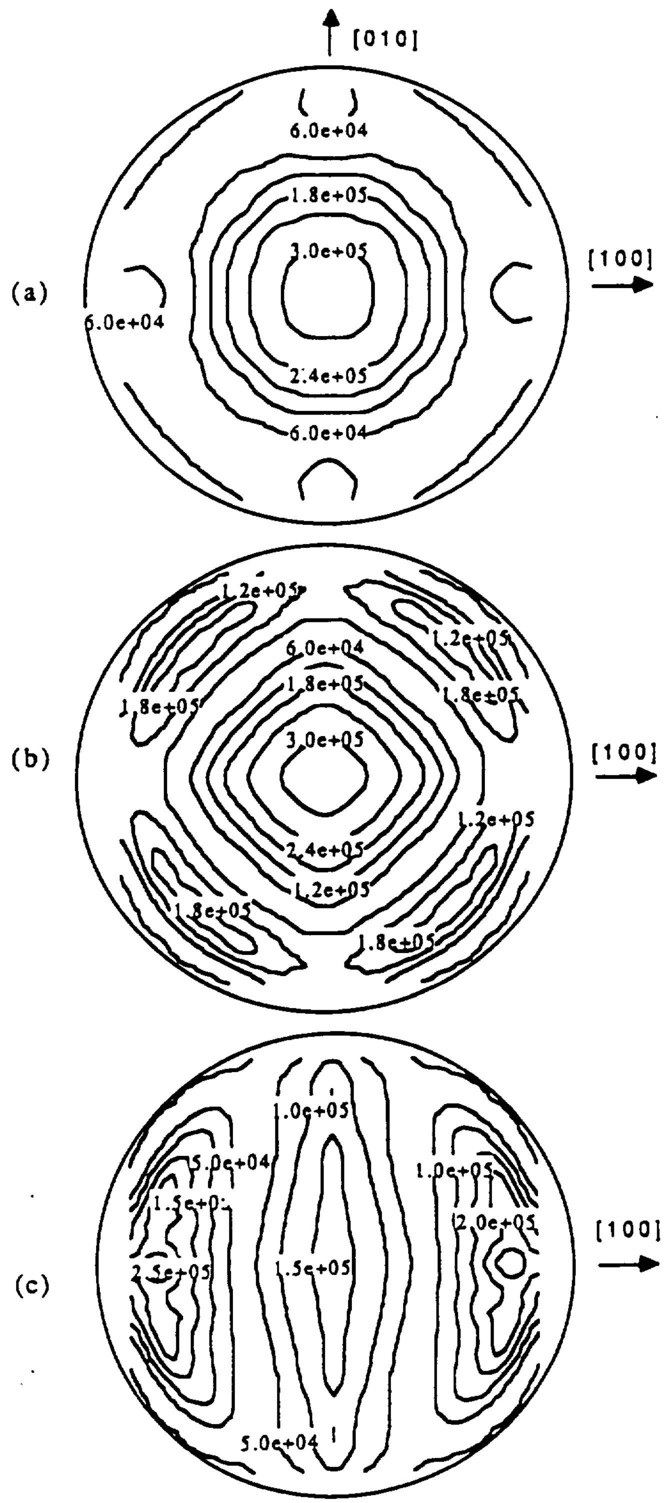


Fig. 5. Resolved shear stresses distribution in the (0 0 1) GaAs wafer near the top of the ingot for (a) (-1 -1 1)[1 1 2], (b) (-1 1 -1)[-1 1 2], and (c) (-1 1 -1)[-2 -1 1] twin systems.

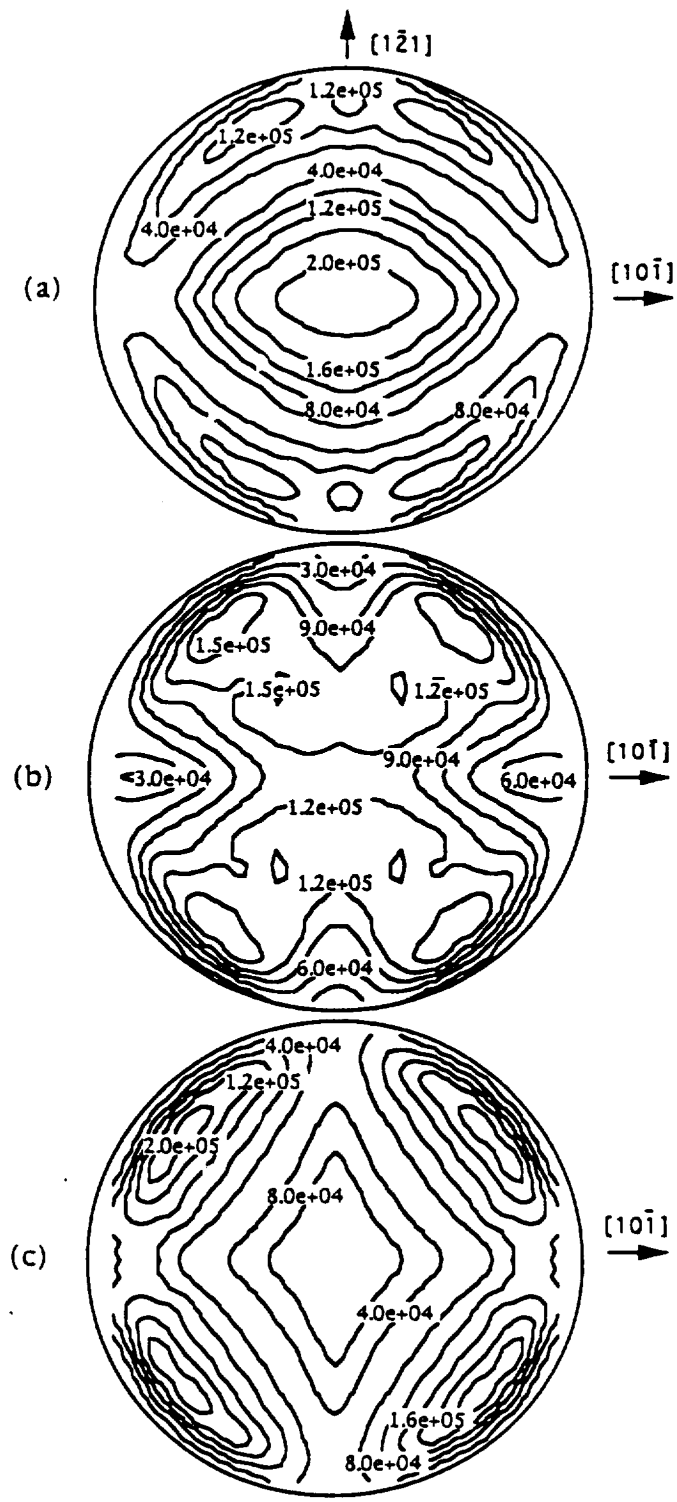


Fig. 6. Resolved shear stresses distribution in the (1 1 1) GaAs wafer near the top of the ingot for (a) (-1 -1 1)[1 1 2], (b) (-1 1 -1)[-1 1 2], and (c) (-1 1 -1)[-2 -1 1] twin systems.